

Microscopic formulas for thermoelectric transport coefficients in lattice systems

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Abstract

A macroscopic description of thermoelectric phenomena involves several tensorial transport coefficients. Textbook microscopic Kubo formulas for them are plagued with ambiguities in the definitions of the current operators and the magnetization. We derive a version of these formulas for lattice systems which is free from ambiguities but contains additional terms compared to the textbook results. For symmetric components of thermoelectric tensors, we identify a large class of lattice systems for which the additional terms vanish with a natural choice of the energy current. To eliminate ambiguities in the skew-symmetric components, one needs to interpret them as relative quantities: only their differences for pairs of materials are well-defined.

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I. INTRODUCTION

Hydrodynamics in a general sense is a coarse-grained description of matter in local thermal equilibrium which incorporates all local conservation laws. It depends on the microscopic details only through transport coefficients. Dissipative transport coefficients such as viscosity, thermal conductivity and electric conductivity are particularly important for applications and their theory is better known. More recently a lot of attention has been devoted to non-dissipative time-reversal-odd transport coefficients such as electric Hall conductivity and Hall viscosity. This interest is explained in part by the contribution that gapless edge modes make to some of these coefficients at low temperatures.

Theoretical studies of transport phenomena often take Kubo formulas as their starting point. These are microscopic formulas for transport coefficients in terms of correlators of currents of conserved quantities. Although Kubo formulas go back to [1, 2] and can be found in many textbooks, there are a number of subtleties in their derivation. It is well appreciated by now that naive Kubo formulas for skew-symmetric parts of the transport tensors must be supplemented with additional terms involving magnetization and "energy magnetization" [3]. Such terms affect thermal Hall conductivity and the skew-symmetric parts of thermoelectric coefficients. Since magnetizations are intrinsically ambiguous, it is not obvious how to evaluate such terms, see [4] for a thorough discussion.

The theory of transport coefficients developed in [2–4] applies to continuum systems. It cannot be directly applied to lattice systems because it assumes certain scaling relations for electric and energy currents which do not hold on a lattice. (In fact, they do not hold for interacting continuum systems either, except after some spatial averaging [3]). Since tight-binding models and other lattice Hamiltonians are ubiquitous in theoretical condensed matter physics, it is important to develop an analogous formalism for them. In [5] we described such a formalism and used it to derive microscopic formulas for the Hall conductivity and thermal Hall conductivity of lattice systems. In this paper we extend it to other transport coefficients. For simplicity, we focus on the case of 2d lattice systems and only briefly discuss the 3d case.

The main results of the paper are as follows. Our formulas for the symmetric parts of conductivity and thermal conductivity tensors [5] are completely analogous to continuum formulas. Surprisingly, this is not the case for the symmetric parts of thermoelectric ten-

sors. In general, microscopic formulas for them contain local terms as well as the expected Kubo term. We show that these extra terms are in fact required to ensure that transport coefficients are unaffected by the ambiguities in the definition of the microscopic energy density. We also show that in special cases, such as systems of free particles or systems with only density-dependent interactions, the additional terms vanish with a natural definition of currents.

The skew-symmetric parts of all transport tensors except conductivity contain contributions from magnetizations. Since magnetizations are defined only up to additive constants, this leads to ambiguities. In the case of thermal conductivity, a way to resolve the ambiguities was described in [5] (building on the results of [3]), and the same approach works for thermoelectric tensors. Namely, although skew-symmetric parts of these tensors are "contaminated" with edge effects, ambiguities cancel when one considers differences of transport tensors for two materials. We express this by saying that skew-symmetric tensors are relative transport coefficients. Microscopic formulas for relative transport coefficients take a more complicated form: they are integrals of differential 1-forms along a path in the space of parameters. These issues do not affect the skew-symmetric part of the conductivity tensor because one can, in principle, measure it in a torus geometry, where no boundaries are present. This is not possible to do even in principle for the skew-symmetric parts of other transport coefficients.

The content of the paper is as follows. In Section II, we explain how ambiguities in definition of transport and magnetization currents leads to a natural separation of transport coefficients into absolute and relative ones. In Section III, we derive microscopic formulas for thermoelectric transport coefficients. We end with a discussion of possible generalizations of our results in Section IV. In one of the appendices, we specialize our formulas to the case of non-interacting fermions and express thermoelectric coefficients in terms of zero-temperature 1-particle Green's functions in coordinate space.

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II. RELATIVE AND ABSOLUTE TRANSPORT COEFFICIENTS

The total current densities are usually divided into two parts:

$$\begin{aligned}\mathbf{j}_{\text{tot}}^N &= \mathbf{j}^N + \mathbf{j}_{\text{mag}}^N, \\ \mathbf{j}_{\text{tot}}^E &= \mathbf{j}^E + \mathbf{j}_{\text{mag}}^E,\end{aligned}\tag{1}$$

where magnetization currents are by definition divergence-free vector fields which do not contribute to net currents across any section of the system. Therefore they must have the form

$$\mathbf{j}_{\text{mag}}^N = \nabla \times \mathbf{M}^N,\tag{2}$$

$$\mathbf{j}_{\text{mag}}^E = \nabla \times \mathbf{M}^E,\tag{3}$$

where $\mathbf{M}^{N,E}$ are defined by these equations and are usually called magnetization density and energy magnetization density, respectively. In the following we will use the same term magnetization for both magnetization and magnetization density which should not lead to a confusion.

The magnetization currents can be present even in an equilibrium state. The transport currents $\mathbf{j}^{N,E}$, on the other hand, can be present only in a non-equilibrium steady state created by slowly varying gradients of external electric potential and temperature (for simplicity of presentation we assume the chemical potential to be constant). This follows from the Bloch theorem [6, 7] and its energy analogue [8]. This constrains the form of transport currents.

Further constraints arise from gauge-invariance. It requires the transport electric current \mathbf{j}^N and the transport “heat current” $\mathbf{j}^E - \varphi \mathbf{j}^N$ to be invariant under shifts of the electrical potential φ by a constant. This follows from the equations defining the current operators $\mathbf{J}^{N,E}(\mathbf{r})$

$$i[H, h(\mathbf{r})] = -\nabla \cdot \mathbf{J}^E(\mathbf{r}), \quad i[H, \rho(\mathbf{r})] = -\nabla \cdot \mathbf{J}^N(\mathbf{r}),\tag{4}$$

and fact that under a constant gauge transformation $\varphi(\mathbf{r}) \mapsto \varphi(\mathbf{r}) + c$ the energy density also transforms as $h(\mathbf{r}) \mapsto h(\mathbf{r}) + c\rho(\mathbf{r})$, where ρ is the electric charge density.

Taking all these considerations into account, one finds that to leading order in the derivative expansion the transport electric current is given by

$$j_k^N = -\sigma_{km} \partial_m \varphi - \nu_{km} \partial_m T,\tag{5}$$

where the conductivity tensor σ_{km} and the thermoelectric tensor ν_{km} are functions of temperature only. For the energy current the expansion is

$$j_k^E = \varphi j_k^N - \eta_{km} \partial_m \varphi - \kappa_{km} \partial_m T. \quad (6)$$

A crucial point for this paper is that the separation of the current densities in (1) is ambiguous. One can always remove a curl of a vector field from $\mathbf{j}^{N,E}$ and add it to $\mathbf{j}_{\text{mag}}^{N,E}$ without affecting the conservation equation and the form of the transport equations (5,6). While this should have no effect on physically observable quantities, it can affect the transport coefficients. Let us specialize to the 2d case and decompose all two-index tensors into symmetric and anti-symmetric parts: $\sigma_{km} = \sigma_{km}^S + \epsilon_{km} \sigma^A$ and similarly for the tensors ν, η , and κ . Taking into account the requirement of gauge-invariance, the allowed redefinitions of the transport currents have the form

$$j_k^N \mapsto j_k^N + \epsilon_{km} \partial_m (\sigma_0 \varphi + f(T)), \quad (7)$$

$$j_k^E \mapsto j_k^E + \epsilon_{km} \partial_m \left(\frac{1}{2} \sigma_0 \varphi^2 + f(T) \varphi + g(T) \right). \quad (8)$$

Here σ_0 is a constant and $f(T), g(T)$ are arbitrary functions of T . Simultaneously magnetizations are redefined as follows:

$$M^N \mapsto M^N - \sigma_0 \varphi - f(T), \quad (9)$$

$$M^E \mapsto M^E - \frac{1}{2} \sigma_0 \varphi^2 - f(T) \varphi - g(T). \quad (10)$$

After the redefinition transport coefficients change:

$$\begin{aligned} \sigma^A &\mapsto \sigma^A - \sigma_0, \\ \nu^A &\mapsto \nu^A - \frac{df(T)}{dT}, \\ \eta^A &\mapsto \eta^A - f(T), \\ \kappa^A &\mapsto \kappa^A - \frac{dg(T)}{dT}. \end{aligned} \quad (11)$$

Using such a redefinition we can always set $\sigma^A(T)$ to vanish at $T = 0$ and make κ^A and η^A vanish identically for any homogeneous material. Instead of setting $\eta^A(T) = 0$, one can choose to set $\nu^A(T) = 0$ and use the remaining freedom to set $\eta^A(0) = 0$. Note also that $\frac{d\sigma^A}{dT}$ and $\nu^A - \frac{d\eta^A}{dT}$ are invariant under such redefinitions.

So far we have ignored the vector potential, or equivalently gauge transformations which depend on the spatial coordinates. Allowing such gauge transformations changes the analysis as follows. Transport electric current \mathbf{j}^N and transport heat current $\mathbf{j}^E - \varphi \mathbf{j}^N$ are now required to depend on φ only through the electric field $E_k = -\partial_k \varphi - \frac{\partial A_k}{\partial t}$. The only difference this makes is that only transformations (7) with $\sigma_0 = 0$ are allowed. As a result, the Hall conductivity σ^A is now free from ambiguities.

There is a natural way to fix ambiguities in M^N and M^E and therefore also in ν^A, η^A and κ^A [3, 5]. If we consider a material with a boundary, the magnetizations as well as all transport coefficients can be set to zero outside. This removes all ambiguities from transport coefficients, but obscures the fact that some transport coefficients are defined relative to vacuum, while others do not depend on any choices and can be measured in the bulk. We will call them relative and absolute transport coefficients, respectively. According to the above analysis, all symmetric transport coefficients as well as σ^A are absolute, while ν^A, η^A , and κ^A are relative. The combination $\nu^A - \frac{d\eta^A}{dT}$ is also absolute.

This distinction has consequences for the microscopic formulas that can be derived for transport coefficients which are usually called Kubo formulas [5]. As we just explained, determination of relative transport coefficients require considering a system with boundaries. On the other hand, as we show in the paper, derivatives of relative transport coefficients with respect to temperature or the parameters of the Hamiltonian involves only correlation functions of a system without boundary. The values of relative transport coefficients for any particular material can be found by integrating this differential over the parameters and/or temperature. The non-uniqueness in the choice of the base point of the integral reflects the ambiguity in the definition of the magnetization currents and can be fixed by choosing the base point to be a trivial insulator. The resulting microscopic formula for a relative transport coefficient is manifestly independent of the choice of boundary conditions at the cost of depending on the correlation functions of a whole family of systems which interpolates between the system of interest and a trivial insulator. On the other hand, microscopic formulas for absolute transport coefficients depend only on the correlation function of the system at a fixed temperature and values of all parameters.

As a consistency check, let us verify that physical bulk quantities depend only on absolute

transport coefficients. For the time derivatives of charge and energy densities we get

$$\frac{\partial \rho^N}{\partial t} = -\nabla \cdot \mathbf{j}^N = -\sigma_{km}^S \partial_k \mathbf{E}_m - \frac{d\sigma_{km}^S}{dT} \mathbf{E}_m \partial_k T - \nu_{km}^S \partial_k \partial_m T - \frac{d\nu_{km}^S}{dT} \partial_k T \partial_m T, \quad (12)$$

$$\begin{aligned} \frac{\partial \rho^E}{\partial t} = -\nabla \cdot \mathbf{j}^E = & -\varphi \nabla \cdot \mathbf{j}^N + \sigma_{km}^S \mathbf{E}_k \mathbf{E}_m - \left(\nu_{km} + \frac{d\eta_{mk}}{dT} \right) \mathbf{E}_k \partial_m T - \eta_{km}^S \partial_k \mathbf{E}_m \\ & + \kappa_{km}^S \partial_k \partial_m T + \frac{d\kappa_{km}^S}{dT} \partial_k T \partial_m T, \end{aligned} \quad (13)$$

where the external fields are assumed to be time-independent and thus $\nabla \times \mathbf{E} = 0$. As expected, these time derivatives are unaffected by the transformations (11).

The time-derivative of entropy density is usually written as follows [9]:

$$\frac{\partial s}{\partial t} = \frac{1}{T} \sigma_{km}^S \mathbf{E}_k \mathbf{E}_m + \frac{1}{T^2} \kappa_{km}^S \partial_k T \partial_m T - \frac{1}{T^2} (T \nu_{km} + \eta_{mk}) \mathbf{E}_k \partial_m T - \nabla \cdot \tilde{\mathbf{j}}_k^S, \quad (14)$$

where the entropy current density is

$$\tilde{\mathbf{j}}_k^S = \frac{1}{T} \eta_{km} \mathbf{E}_m - \frac{1}{T} \kappa_{km}^S \partial_m T. \quad (15)$$

The r.h.s. of eq. (14) seems to depend on some relative transport coefficients. However, if one redefines the entropy current as follows:

$$\mathbf{j}_k^S = \frac{1}{T} \eta_{km}^S \mathbf{E}_m - \frac{1}{T} \kappa_{km}^S \partial_m T, \quad (16)$$

then one can write

$$\frac{\partial s}{\partial t} = \frac{1}{T} \sigma_{km}^S \mathbf{E}_k \mathbf{E}_m + \frac{1}{T^2} \kappa_{km}^S \partial_k T \partial_m T - \frac{1}{T^2} \left(T \nu_{km}^S + \eta_{mk}^S + \epsilon_{km} T \left(\nu^A - \frac{d\eta^A}{dT} \right) \right) \mathbf{E}_k \partial_m T - \nabla \cdot \mathbf{j}_k^S. \quad (17)$$

It is manifest now that both the entropy production rate and the entropy current depend only on the absolute transport coefficients.

Since only absolute transport coefficients enter the expressions for the divergences of currents, measuring net currents through closed curves (or surfaces, if we are discussing a 3d material) does not allow to determine relative transport coefficients. This applies even to infinite curves with a boundary at infinity, provided φ and T tend to fixed values at infinity. The latter condition must be imposed to eliminate the contribution of magnetization currents. For example, if we compute the electric current I_x^N through a vertical line $x = 0$, then the contribution of ν^A drops out because

$$\int_{-\infty}^{\infty} dy \nu^A \partial_y T dy = 0. \quad (18)$$

The above considerations apply to a homogeneous material whose transport coefficients are constants. If one considers a heterogeneous material, such as an interface between two homogeneous ones, then the expressions for net currents will involve differences between relative transport coefficients. For example, consider a sample such that ν^A interpolates between ν_1^A for $y \ll 0$ and ν_2^A for $y \gg 0$. Suppose that the temperature is a function of y only which is equal to T_b throughout the interface region and approaches T_∞ at $y \rightarrow \pm\infty$. Then the ν^A -dependent contribution to the net electric current in the x direction is

$$-\int_{-\infty}^{\infty} dy \nu^A \partial_y T = (T_b - T_\infty)(\nu_2^A - \nu_1^A), \quad (19)$$

Similarly, the contribution of κ^A to the net heat current is $(T_b - T_\infty)(\kappa_2^A - \kappa_1^A)$. By creating an electric potential φ which is equal to φ_b in the interface region and approaches φ_∞ at $y \rightarrow \pm\infty$, one can also measure $\sigma_2^A - \sigma_1^A$ and $\eta_2^A - \eta_1^A$.

In the case of the electric Hall conductivity one can do better by utilizing a time-dependent vector potential rather than a scalar potential and working in a cylinder geometry or a torus geometry. Then in principle one can determine σ^A for a single material by measuring the net flow of electric charge across a section of a cylinder or a torus as one inserts a unit of magnetic flux through this section. This does not work for η^A because the physical quantity that needs to be measured is the net amount of heat transferred to the heat bath as one inserts a unit of magnetic flux (see Fig. 1). Therefore heat transport will receive a contribution from the work of the electromotive force \mathcal{E} on the net electric edge currents I_{edge}^N . The edge currents are proportional to the jump in the magnetization along the boundary and they make η^A relative even in the cylinder geometry.

III. MICROSCOPIC FORMULAS FOR THERMOELECTRIC COEFFICIENTS

A. Currents on a lattice

We follow the conventions of [5]. We consider a lattice system with a Hamiltonian $H = \sum_{p \in \Lambda} H_p$, where $\Lambda \subset \mathbb{R}^2$ is a not necessarily regular lattice. The operators H_p have a finite range, i.e. there exist R such that H_p acts trivially on site q if $|p - q| > R$. The space of states at each site of the lattice is assumed to be finite-dimensional. The electric charge operator Q has the form $Q = \sum_{p \in \Lambda} Q_p$, where Q_p has integral eigenvalues (we set the electric

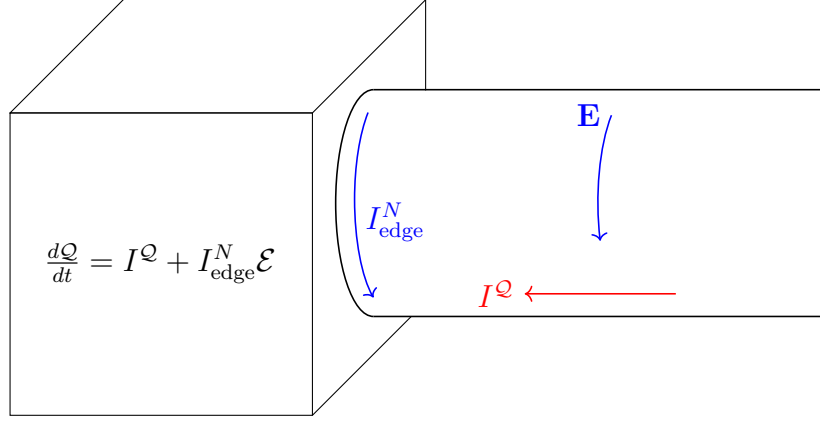


FIG. 1: Insertion of a flux Φ into a cylinder creates electric field around it. If $\eta_{xy} \neq 0$, this electric field \mathbf{E} drives a heat current I^Q along the axis of the cylinder. The jump of the magnetization gives rise to an edge current I_{edge}^N . Work done on the edge current by the electric field contributes to the net heat Q transferred to the heat bath.

charge of electron to be 1) and acts only on site p . This means that the $U(1)$ symmetry is on-site. In particular, $[Q_p, Q_q] = 0$ for all $p, q \in \Lambda$.

The electric current from site q to site p is defined as

$$J_{pq}^N = i[H_q, Q_p] - i[H_p, Q_q]. \quad (20)$$

The energy current from site q to site p is defined as

$$J_{pq}^E = -i[H_p, H_q]. \quad (21)$$

These currents enter the charge and energy conservation equations

$$\frac{dQ_q}{dt} = i \sum_{p \in \Lambda} [H_p, Q_q] = - \sum_{p \in \Lambda} J_{pq}^N, \quad (22)$$

$$\frac{dH_q}{dt} = i \sum_{p \in \Lambda} [H_p, H_q] = - \sum_{p \in \Lambda} J_{pq}^E. \quad (23)$$

The net current from a subset $B \subset \Lambda$ to its complement $A = \Lambda \setminus B$ is given by

$$J^{N,E}(A, B) = \sum_{p \in A} \sum_{q \in B} J_{pq}^{N,E}. \quad (24)$$

This observable measures the net current across the boundary of A and B . In this paper we will need its mild generalization. For a given skew-symmetric function $\eta(p, q) : \Lambda \times \Lambda \rightarrow \mathbb{R}$ satisfying

$$\eta(p, q) + \eta(q, r) + \eta(r, p) = 0, \quad \forall p, q, r \in \Lambda, \quad (25)$$

define

$$J^{N,E}(\eta) = \frac{1}{2} \sum_{p,q \in \Lambda} \eta(p,q) J_{pq}^{N,E}. \quad (26)$$

Current $J(A, B)$ from B to $A = \Lambda \setminus B$ corresponds to the case $\eta(p, q) = \chi_B(q) - \chi_B(p)$, where the function $\chi_B(p)$ is equal 1 on B and 0 otherwise.

The equilibrium expectation value of the currents satisfy

$$\sum_{p \in \Lambda} \langle J_{pq}^{N,E} \rangle = 0. \quad (27)$$

This equation is a lattice analog of the continuum equation

$$\nabla \cdot \langle \mathbf{J}^{N,E}(\mathbf{r}) \rangle = 0. \quad (28)$$

In the continuum the general solution to this equation

$$\langle J_k^{N,E}(\mathbf{r}) \rangle = -\epsilon_{kj} \partial_j M^{N,E}(\mathbf{r}) \quad (29)$$

defines the magnetization M^N and energy magnetization M^E . Analogously, on a lattice the solution of equation (27) is

$$\langle J_{qr}^{N,E} \rangle = \sum_{p \in \Lambda} M_{pqr}^{N,E}, \quad (30)$$

where $M_{pqr}^{N,E}$ are skew-symmetric functions of the lattice points $p, q, r \in \Lambda$. These are lattice analogs of the magnetization and the energy magnetisation. Physically, in continuum case $M^{N,E}(r)$ represent the circulating currents of the system in equilibrium. Similarly, $M_{pqr}^{N,E}$ physically can be thought as quantity which measures the circulating current around a triangle formed by p, q, r .

Unfortunately, $M_{pqr}^{N,E}$ is not unique: one can always redefine

$$M_{pqr}^{N,E} \mapsto M_{pqr}^{N,E} + \sum_{s \in \Lambda} N_{pqrs}, \quad (31)$$

where N_{pqrs} is skewsymmetric function of its subscripts which decays whenever any two of them are far apart. This corresponds to ambiguity in splitting of the circulating currents into contributions of magnetization from the different triangles and it is absent in continuum case.

There is an additional ambiguity corresponding to existence of solutions to the equation $\sum_{r \in \Lambda} M_{pqr}^{N,E} = 0$ which are not of the form $\sum_{s \in \Lambda} N_{pqrs}$. It corresponds to an ambiguity of

addition of a constant to the magnetization in continuum case. A standard method to deal with the later is to consider a system with a boundary and fix the magnetization to be zero outside of the system. In this paper, we want to think about all transport coefficients as manifestly bulk quantities and avoid dealing with boundaries. While magnetization itself suffers from ambiguities and depends non-locally on the boundary conditions, the variation of magnetization with respect to parameters of the Hamiltonian is local. Indeed, consider the variation of the equation (30) with respect to a parameter λ^ℓ of the Hamiltonian

$$\frac{\partial}{\partial \lambda^\ell} \langle J_{pq}^{N,E} \rangle = \sum_{r \in \Lambda} \mu_{pqr,\ell}^{N,E}, \quad (32)$$

where $\mu_{pqr,\ell}^{N,E} = \frac{\partial M_{pqr}^{N,E}}{\partial \lambda^\ell}$ and is given by [10]

$$\mu_{pqr,\ell}^{N,E} = -\beta \langle \langle \frac{\partial H_p}{\partial \lambda^\ell}; J_{qr}^{N,E} \rangle \rangle - \beta \langle \langle \frac{\partial H_r}{\partial \lambda^\ell}; J_{pq}^{N,E} \rangle \rangle - \beta \langle \langle \frac{\partial H_q}{\partial \lambda^\ell}; J_{rp}^{N,E} \rangle \rangle, \quad (33)$$

where $\langle \langle A; B \rangle \rangle$ denotes the Kubo canonical pairing [1]. Using the properties of the Kubo pairing (see Appendix A), one can easily verify the identity (32). In the following we will combine derivatives of magnetizations with respect to different parameters into 1-forms on the parameter space $\mu_{pqr}^{N,E} = \sum_\ell \mu_{pqr,\ell}^{N,E} d\lambda^\ell$.

B. Equilibrium conditions and driving forces

In the following sections we will follow Luttinger [2] and study the behavior of the system coupled to external potentials

$$H_p^{\psi,\varphi} = (1 + \psi(p))(H_p + \varphi(p)Q_p), \quad (34)$$

where $\varphi(p)$ is external electric potential and $\psi(p)$ can be thought of as gravitational potential. The potentials are assumed to infinitesimally small slowly-varying functions of p which vanish at infinity. After coupling to external potentials the system will eventually relax into a state with density matrix

$$\rho \sim \exp \left(-\frac{H^{\psi,\varphi} - \mu_0 Q}{T_0} \right), \quad (35)$$

where T_0 and μ_0 are the temperature and local chemical potential of the system at infinity. On the other hand, on physical grounds we expect local observables supported in some small

but macroscopic region around site p to be described by a thermal density matrix

$$\rho(p) \sim \left(-\frac{H - \mu(p)Q}{T(p)} \right), \quad (36)$$

where the local temperature $T(p)$ and chemical potential $\mu(p)$ are slowly varying functions of p . The equilibrium conditions can be found to be [2–4]

$$(1 + \psi(p))(\mu(p) + \varphi(p)) = \mu_0, \quad (37)$$

$$(1 + \psi(p))T(p) = T_0. \quad (38)$$

These relations together with the absence of transport currents in equilibrium can be used to derive Einstein relations between transport coefficients [2]. The latter also leads to transport currents being proportional to the gradients of the left hand sides of eqs. (37) and (38). The fact that the driving forces depend only on specific combinations of ψ, φ, T, μ will be used to relate the response to variations of the thermodynamic parameter T to the response to variations of the external field ψ .

Note that, in section II for simplicity we assumed that chemical potential is constant. We will continue doing so in the rest of the paper and we will assume $\mu(p)$ to be constant. Generalization to a more general case of non-constant local chemical potential is straightforward, but clumsy due to ambiguities in the separation of electrochemical potential $\mu + \varphi$ into two parts.

C. Nernst effect

In order to find the thermoelectric coefficient ν_{xy} we deform the Hamiltonian density by

$$\Delta H_p = \epsilon e^{st} \widehat{g}(p) H_p, \quad (39)$$

where $\widehat{g}(p)$ is a hat-shaped function as in Fig. 2b, ϵ is an infinitesimal parameter, and s is a small positive number which controls how fast the perturbation is turned on. We will consider the so-called fast regime [2] in which the characteristic time $1/s$ is large but not large enough in order for the two slopes of the hat $\widehat{g}(p)$ to come into equilibrium.

The change of the state of the system can be found as follows. The density matrix

$$\rho(t) = \rho_0 + \Delta\rho(t) \quad (40)$$

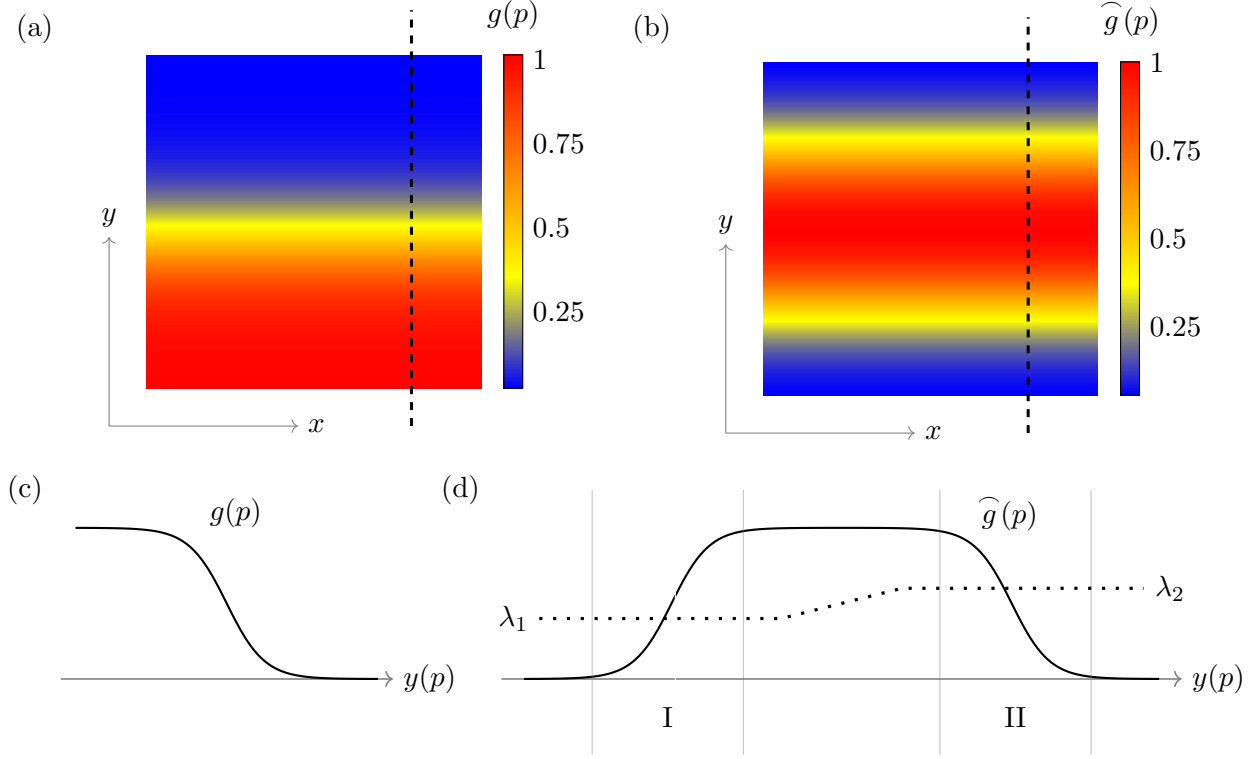


FIG. 2: (a) Heat map of the function $g(p)$ corresponding to a temperature gradient in a horizontal strip. (b) Heat map of the function $\widehat{g}(p)$ corresponding to two horizontal strips with the opposite signs of the temperature gradient. (c) The function $g(p)$ restricted to the dashed line in (a). (d) The function $\widehat{g}(p)$ restricted to the dashed line in (b). Dotted line in (d) represents the dependence of some parameter λ of the Hamiltonian on $y(p)$.

satisfies the quantum Liouville equation

$$\frac{d\Delta\rho}{dt} = -i[\Delta H, \rho_0] + \dots, \quad (41)$$

where ρ_0 is the equilibrium density matrix at $t = -\infty$ and dots represent higher order terms in ϵ . The solution to this equation is

$$\Delta\rho(t=0) = -\rho_0 \int_0^\infty dt \int_0^\beta d\tau \Delta \dot{H}(-t - i\tau), \quad (42)$$

where the dot denotes the time derivative. The change of the observable A can be found to be

$$\Delta\langle A \rangle = \langle \Delta A \rangle - \beta \int_0^\infty dt \langle \langle A; \Delta \dot{H}(-t) \rangle \rangle, \quad (43)$$

where we used the Kubo pairing notation (see Appendix A) and ΔA is the variation of the operator arising from explicit dependence of A on the Hamiltonian. Using explicit form of

the perturbation (39), energy conservation law and properties of the Kubo pairing we can rewrite this formula as

$$\Delta\langle A \rangle = \langle \Delta A \rangle + \epsilon\beta \int_0^\infty dt e^{-st} \langle \langle A(t); J^E(\delta\widehat{g}) \rangle \rangle, \quad (44)$$

where we neglected term proportional to small s .

The change in the electric current across a vertical line $x = a$ is

$$\Delta\langle J^N(\delta f) \rangle = \langle \Delta J^N(\delta f) \rangle + \epsilon\beta \int_0^\infty dt e^{-st} \langle \langle J^N(\delta f, t); J^E(\delta\widehat{g}) \rangle \rangle, \quad (45)$$

where $f(p) = \theta(a - x(p))$ is a step function. The explicit variation of the current is

$$\begin{aligned} \langle \Delta J^N(\delta f) \rangle &= \frac{i\epsilon}{2} \sum_{p,q \in \Lambda} \langle \widehat{g}(q)[H_q, Q_p] - \widehat{g}(p)[H_p, Q_q] \rangle (f(q) - f(p)) \\ &= \frac{\epsilon}{4} \sum_{p,q \in \Lambda} \langle J_{pq}^N \rangle (\widehat{g}(p) + \widehat{g}(q)) (f(q) - f(p)) \\ &\quad + \frac{i\epsilon}{4} \sum_{p,q \in \Lambda} \langle [H_q, Q_p] + [H_p, Q_q] \rangle (f(q) - f(p)) (\widehat{g}(q) - \widehat{g}(p)), \end{aligned} \quad (46)$$

where in the last line we separated the result into two contribution formally skew-symmetric and symmetric in f, \widehat{g} . The second term depends only on difference of values of \widehat{g} at different sites as expected for a transport current. On the other hand, the first term depends on the value of \widehat{g} and does not seem to be of the form expected for a transport current. As was explained in [3] this contribution is related to magnetization currents. Indeed we can rewrite

$$\frac{\epsilon}{4} \sum_{p,q \in \Lambda} \langle J_{pq}^N \rangle (\widehat{g}(p) + \widehat{g}(q)) (f(q) - f(p)) = \sum_{p,q,r \in \Lambda} M_{pqr}^N (f(q) - f(p)) (\widehat{g}(q) - \widehat{g}(r)), \quad (47)$$

where we used skew-symmetry of M_{pqr}^N .

Written in this form, the response is proportional to the differences of \widehat{g} at different points and therefore receives appreciable contributions only from regions *I* and *II* in Fig. 2d. However, the transformation (47) contains an important subtlety. The right-hand side hand side contains a magnetization contribution which is ambiguously defined while left-hand side is unambiguous. There is no contradiction because the ambiguity in the region *I* will compensate the one in the region *II*. Moreover, in a homogeneous system the response will be zero, because these two regions compensate each other exactly. One way to deal with it is to introduce a boundary somewhere in between the two regions and enforce the magnetization M to be 0 outside of the sample. This approach is used in [3] in the continuum

case. However, an explicit boundary introduces additional computational challenges and makes the bulk nature of the Nernst effect obscure.

In this paper, we will use an alternative approach proposed in [5]. Instead of introducing a sharp boundary, we will make one parameter of the Hamiltonian λ to have slightly different values in regions I and II (see Fig. 2d). We can write the hat-shaped function \widehat{g} as a difference of two functions g_I and g_{II} , $\widehat{g}(p) = g_{II}(p) - g_I(p)$, each of which is a translate of the function $g(p)$ which depends only on $y(p)$ and is shown in Fig. 2c. The functions $g_{I,II}$ are non-constant only in regions I and II respectively. Then the magnetization contribution can be rewritten as

$$\epsilon(\lambda_{II} - \lambda_I)\mu_\lambda^N(\delta g \cup \delta f) + O((\lambda_{II} - \lambda_I)^2), \quad (48)$$

where $\mu_{pqr,\lambda}^N = \frac{\partial M_{pqr}^N}{\partial \lambda}$, and we introduced a notation

$$\mu_\lambda^N(\delta f_1 \cup \delta f_2) = \frac{1}{6} \sum_{p,q,r \in \Lambda} \mu_{pqr,\lambda}^N (f_1(q) - f_2(p))(f_2(r) - f_2(q)). \quad (49)$$

Combining this with other contributions we find

$$\delta \langle J^N(\delta f) \rangle \approx \epsilon(\lambda_{II} - \lambda_I) \left\{ \frac{\partial}{\partial \lambda} \left[\beta \int_0^\infty dt e^{-st} \langle \langle J^N(\delta f, t); J^E(\delta g) \rangle \rangle + U(\delta f, \delta g) \right] + \mu_\lambda^N(\delta g \cup \delta f) \right\}, \quad (50)$$

where

$$U(\delta f, \delta g) = \frac{i}{4} \sum_{p,q \in \Lambda} \langle [H_q, Q_p] + [H_p, Q_q] (f(q) - f(p))(g(q) - g(p)) \rangle. \quad (51)$$

The function g as in Fig. 2c is not compactly supported and thus it takes an infinite time for the system to equilibrate. Therefore, one can take the limit $s \rightarrow 0$ while staying in the “fast” regime. From eqs. (37,38) one finds that electric current after perturbation by gravitational potential $\epsilon g(p)$ is equal to the current generated by

$$T(p) = \epsilon g(p) T_0, \quad (52)$$

$$\varphi(p) = \epsilon g(p) \mu_0. \quad (53)$$

From continuum phenomenological equation (5) one finds the current across $x = a$ line to be

$$- \epsilon T_0 \int_{-\infty}^{\infty} \nu_{xy} \partial_y g dy - \epsilon \mu_0 \int_{-\infty}^{\infty} \sigma_{xy} \partial_y g dy = \epsilon T_0 \int_{\lambda_I}^{\lambda_{II}} \frac{\partial \nu_{xy}}{\partial \lambda} d\lambda + \epsilon \mu_0 \int_{\lambda_I}^{\lambda_{II}} \frac{\partial \sigma_{xy}}{\partial \lambda} d\lambda. \quad (54)$$

Comparing it to (50) we find

$$d\nu_{xy} = d\left[\beta^2 \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle J^N(\delta f, t); J^Q(\delta g) \rangle + \beta U(\delta f, \delta g)\right] - \beta \mu^N(\delta f \cup \delta g), \quad (55)$$

where we introduced the notation $J^Q = J^E - \mu J^N$ for the heat current, inverse temperature $\beta = \frac{1}{T}$, we dropped the subscript 0 from T_0 and μ_0 since this formula contains correlation functions of the unperturbed system in equilibrium. We combined differential with respect to parameter into the differential form $\mu^N(\delta f \cup \delta g) = \mu_\lambda^N(\delta f \cup \delta g) d\lambda$ and the derivation can be straightforwardly extended to involve several parameters. The exterior derivative $d = \sum_\ell d\lambda \frac{\partial}{\partial \lambda^\ell}$ acts on the parameter space.

Since rescaling the temperature is equivalent to rescaling the Hamiltonian, we can extend this 1-form to the enlarged parameter space which includes T . Then we can define the difference of coefficients η_{xy} for any two 2d materials, regardless of the temperature. Explicitly, let us define the rescaled Hamiltonian $H_{\lambda_0} = \lambda_0 H$, where we introduced an additional scaling parameter λ_0 . Then

$$\left(T \frac{\partial}{\partial T} + \lambda_0 \frac{\partial}{\partial \lambda_0} \Big|_{\lambda_0=1}\right) \nu_{xy}(\lambda_0, T) = 0. \quad (56)$$

Therefore we can define the T -component of the 1-form on the enlarged parameter space as follows:

$$\frac{d\nu_{xy}}{dT} = \frac{\partial}{\partial T} \left[\beta^2 \int_0^\infty dt e^{-st} \langle J^N(\delta f, t); J^Q(\delta g) \rangle + \beta U(\delta f, \delta g) \right] - \beta^2 \tau^N(\delta f \cup \delta g), \quad (57)$$

where $\tau^N(\delta f \cup \delta g)$ is given by eq. (49) with μ_{pqr} replaced with

$$\tau_{pqr}^N = \beta \langle \langle H_p; J_{qr}^N \rangle \rangle + \beta \langle \langle H_r; J_{pq}^N \rangle \rangle + \beta \langle \langle H_q; J_{rp}^N \rangle \rangle, \quad (58)$$

which is obtained from μ^N by replacing dH_p with $-H_p$.

D. Ettingshausen effect

One can derive a formula for the coefficient η_{xy} in a similar way. In this section, we will display only the key steps, since all arguments are the same.

In order to find the coefficient we deform the Hamiltonian density by

$$\Delta H_p = \epsilon e^{st} \widehat{g}(p) Q_p, \quad (59)$$

where $\widehat{g}(p)$ is a hat-shaped function of $y(p)$ as in Fig. 2b.

The change in the energy current across a vertical line $x = a$ is

$$\Delta\langle J^E(\delta f) \rangle = \langle \Delta J^E(\delta f) \rangle + \epsilon\beta \int_0^\infty dt e^{-st} \langle \langle J^E(\delta f, t); J^N(\delta \widehat{g}) \rangle \rangle, \quad (60)$$

where $f = \theta(a - x(p))$. The explicit variation of the current is

$$\begin{aligned} \langle \Delta J^E(\delta f) \rangle &= \frac{i\epsilon}{2} \sum_{p,q \in \Lambda} \langle \widehat{g}(p)[H_q, Q_p] - \widehat{g}(q)[H_p, Q_q] \rangle (f(q) - f(p)) \\ &= \frac{\epsilon}{4} \sum_{p,q \in \Lambda} \langle J_{pq}^N \rangle (\widehat{g}(p) + \widehat{g}(q)) (f(q) - f(p)) - U(\delta f, \delta \widehat{g}), \end{aligned} \quad (61)$$

The first term can be expressed in terms of magnetization as in (47). We write $\widehat{g}(p)$ as a difference $\widehat{g}(p) = g_{II}(p) - g_I(p)$, where $g_{I,II}$ are translates of a smeared step-function $g(p)$. Then we rewrite the response as a difference of conductivities of different materials:

$$\delta\langle J^E(\delta f) \rangle \approx \epsilon(\lambda_{II} - \lambda_I) \left\{ \frac{\partial}{\partial \lambda} \left[\beta \int_0^\infty dt e^{-st} \langle \langle J^E(\delta f, t); J^N(\delta g) \rangle \rangle - U(\delta f, \delta g) \right] + \mu_\lambda^N(\delta g \cup \delta f) \right\}. \quad (62)$$

On the other hand, from the continuum phenomenological equation (6) one finds the current across the line $x = a$ to be

$$- \epsilon \int_{-\infty}^\infty \eta_{xy} \partial_y g dy - \epsilon \mu \int_{-\infty}^\infty \sigma_{xy} \partial_y g dy = \epsilon \int_{\lambda_I}^{\lambda_{II}} \frac{\partial \eta_{xy}}{\partial \lambda} d\lambda + \epsilon \mu \int_{\lambda_I}^{\lambda_{II}} \frac{\partial \sigma_{xy}}{\partial \lambda} d\lambda, \quad (63)$$

where the second term originates from the contribution of $\varphi \mathbf{j}^N$ to \mathbf{j}^E . Comparing it to (62) we find

$$d\eta_{xy} = d \left[\beta \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle \langle J^Q(\delta f, t); J^N(\delta g) \rangle \rangle - U(\delta f, \delta g) \right] - \beta \mu^N(\delta f \cup \delta g). \quad (64)$$

This 1-form can be extended to include temperature as a parameter using the scaling relation

$$\left(T \frac{\partial}{\partial T} + \lambda_0 \frac{\partial}{\partial \lambda_0} \Big|_{\lambda_0=1} \right) \frac{\eta_{xy}(\lambda_0, T)}{T} = 0. \quad (65)$$

Therefore we can define the T -component of the 1-form on the enlarged parameter space as follows:

$$\frac{d}{dT} \frac{\eta_{xy}}{T} = \frac{\partial}{\partial T} \left[\beta^2 \int_0^\infty dt e^{-st} \langle \langle J^Q(\delta f, t); J^N(\delta g) \rangle \rangle - \beta U(\delta f, \delta g) \right] - \beta^2 \tau^N(\delta f \cup \delta g), \quad (66)$$

where τ^N is given by (58).

E. Symmetric parts of transport coefficients

Note that the 1-forms $\mu^N(\delta f \cup \delta g)$ and $\tau^N(\delta f \cup \delta g)$ are formally skew-symmetric under the exchange of f and g . To make use of this symmetry, we need to argue that f can be replaced with a smeared step-function in the x direction. This can be argued using matching between microscopic theory and hydrodynamics. Namely, we expect that the microscopic linear response can be used to compute the properties of a Non-Equilibrium Steady State (NESS). Replacing f with a smeared step-function changes the operators $J^N(\delta f)$ and $J^E(\delta f)$ by $J^N(\widehat{\delta f})$ and $J^E(\widehat{\delta f})$. The latter operators can be equivalently written as $\frac{dQ(\widehat{f})}{dt}$ and $\frac{dH(\widehat{f})}{dt}$, where

$$Q(\widehat{f}) = \sum_{p \in \Lambda} \widehat{f}(p) Q_p, \quad H(\widehat{f}) = \sum_{p \in \Lambda} \widehat{f}(p) H_p, \quad (67)$$

and $\widehat{f}(p)$ is a hat-shaped function which depends only on $x(p)$. On the other hand, if the microscopic linear response is to reproduce the expected properties of a NESS, the expectation value of these observables must be zero. Thus we can replace f with a smeared step-function in the x -direction without affecting ν_{xy} or η_{xy} .

After this has been done, exchanging f and g is equivalent to exchanging x and y . Thus $\mu^N(\delta f \cup \delta g)$ does not enter the microscopic formulas for the symmetrized thermoelectric coefficients. These formulas then can be integrated, giving

$$\nu_{xy}^S = \frac{\beta^2}{2} \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} [\langle \langle J^N(\delta f, t); J^Q(\delta g) \rangle \rangle + \langle \langle J^N(\delta g, t); J^Q(\delta f) \rangle \rangle] + \beta U(\delta f, \delta g), \quad (68)$$

$$\eta_{xy}^S = \frac{\beta}{2} \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} [\langle \langle J^Q(\delta f, t); J^N(\delta g) \rangle \rangle + \langle \langle J^Q(\delta g, t); J^N(\delta f) \rangle \rangle] - U(\delta f, \delta g). \quad (69)$$

As we show in Appendix C, the two terms on the right-hand side of these equation are not separately invariant under Hamiltonian density redefinition, but the full transport coefficients are invariant. The correction term $U(\delta f, \delta g)$ is zero for fermionic systems with only density-dependent interactions (see Appendix D for more details).

F. Skew-symmetric parts of transport coefficients

In a similar way one can find skew-symmetric parts of transport coefficients

$$d\nu^A = d \left[\frac{\beta^2}{2} \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \left(\langle \langle J^N(\delta f, t); J^Q(\delta g) \rangle \rangle - \langle \langle J^N(\delta g, t); J^Q(\delta f) \rangle \rangle \right) \right] - \beta \mu^N(\delta f \cup \delta g), \quad (70)$$

$$d\eta^A = d \left[\frac{\beta}{2} \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \left(\langle \langle J^Q(\delta f, t); J^N(\delta g) \rangle \rangle - \langle \langle J^Q(\delta g, t); J^N(\delta f) \rangle \rangle \right) \right] - \beta \mu^N(\delta f \cup \delta g). \quad (71)$$

These formulas give only derivatives of transport coefficients with respect to parameters. Integration of these formulas over parameters or temperature gives the difference of relative transport coefficients at different values of parameters. It is natural to define relative transport coefficients of a trivial insulator to be zero. Determination of the relative transport coefficient in this case would correspond to integration over a path in the parameter space from a trivial insulator to the material of interest.

There are many paths which one can use to deform a system into a trivial one. Consistency requires the integral of $d\nu^A$ or $d\eta^A$ to depend only on the endpoints of the path. This means that the 1-form $\mu^N(\delta f \cup \delta g)$ must be exact. This can be proved using the techniques of [5] where $\mu^E(\delta f \cup \delta g)$ was shown to be exact.

IV. DISCUSSION

In this paper we have derived microscopic formulas for “transverse” thermoelectric coefficients of general 2d lattice systems. It was convenient to decompose them into symmetric and anti-symmetric parts, since they have qualitatively different behavior: the former are absolute transport coefficients, while the latter are relative. Similar formulas for electric Hall conductivity and thermal Hall conductivity have already been derived in [5].

The usual Kubo formulas for transport coefficients require averaging the correlators of currents over the whole space. In contrast, our microscopic formulas involve net currents through two perpendicular lines. This is because a current on a 2d lattice is a function of a pair of points, and the natural observable associated to it is localized on a line rather than at a point. Despite this, after the limit $s \rightarrow 0$ has been taken, our formula computes the same quantity as the usual continuum Kubo formula.

It is natural to ask whether longitudinal components of conductivity, thermal conductivity, and thermoelectric tensors of a 2d lattice system can be computed in a similar manner. This is easily achieved: one simply replaces two perpendicular lines with two lines making a nonzero angle θ . It is easy to see determine from hydrodynamics which linear combination of components of the transport tensors describes the corresponding linear response. For example, if both currents involved are electric currents, one of the lines is given by $y = 0$, and the other one is $y = x \cdot \tan \theta$, then the correlator

$$\beta \lim_{s \rightarrow 0+} \int_0^\infty e^{-st} \langle \langle J^N(\delta f, t); J^N(\delta g) \rangle \rangle dt \quad (72)$$

measures $\sigma_{xy} - \frac{1}{\tan \theta} \sigma_{yy}$. Thus by changing the functions f, g one can extract all four components of the conductivity tensor. The same is true about other transport coefficients.

In this paper we focused on the case of 2d materials, but the 3d case can be accommodated as well. One can simply replace a lattice in \mathbb{R}^2 with a lattice in $\mathbb{R}^2 \times [0, L]$, impose periodic boundary conditions in the third direction, divide all formulas by L , and take the limit $L \rightarrow \infty$. The functions f, g remain independent of the third coordinate. It should not matter whether the limit $L \rightarrow \infty$ is taken before or after the limit $s \rightarrow 0$, since the problem is translationally invariant in the third direction.

In the 2d case, the quantity $\nu^A(T)$ (normalized relative to the vacuum) is dimensionless, and Bloch's theorem implies that for gapped systems $\nu^A(0)$ does not change under the variations of the Hamiltonian which do not close the gap. Thus if $\nu^A(0)$ were nonzero, it would represent a new topological invariant of gapped 2d phases of matter. However, one can show that on very general grounds $\nu^A(0)$ vanishes for all gapped systems [11]. By Onsager reciprocity, the $T \rightarrow 0$ limit of $\eta^A(T)/T$ also vanishes. Thus topological invariants of gapped 2d systems arise only from the Hall conductivity and the thermal Hall conductivity.

Appendix A: Kubo canonical pairing

Kubo canonical pairing of two operators A, B is defined as follows:

$$\langle \langle A; B \rangle \rangle = \frac{1}{\beta} \int_0^\beta \langle A(-i\tau) B \rangle d\tau - \langle A \rangle \langle B \rangle. \quad (A1)$$

Here $\langle \dots \rangle$ denotes average over a Gibbs state at temperature $T = 1/\beta$ (or more generally, over a state satisfying the Kubo-Martin-Schwinger condition), and $A(-i\tau) = e^{H\tau} A e^{-H\tau}$.

Kubo pairing determines static linear response: if the Hamiltonian is perturbed by λB , where λ is infinitesimal, then the change in the expectation value of A due to the change in the equilibrium density matrix is

$$\Delta\langle A \rangle = -\beta\lambda\langle\langle A; B \rangle\rangle. \quad (\text{A2})$$

Kubo pairing is symmetric, $\langle\langle A; B \rangle\rangle = \langle\langle B; A \rangle\rangle$, and satisfies

$$\beta\langle\langle i[H, A]; B \rangle\rangle = \langle i[B, A] \rangle. \quad (\text{A3})$$

In finite volume, one can write it in terms of the energy eigenstates as follows:

$$\langle\langle A; B \rangle\rangle = Z^{-1} \sum_{n,m} \langle n|\bar{A}|m\rangle \langle m|\bar{B}|n\rangle \frac{e^{-\beta E_m} - e^{-\beta E_n}}{\beta(E_n - E_m)}, \quad (\text{A4})$$

where $\bar{A} = A - \langle A \rangle$, and $\bar{B} = B - \langle B \rangle$.

Appendix B: Onsager reciprocity revisited

Derivations of Onsager relations are based on the analysis of hydrodynamic fluctuations, so it might seem that they should put constraints only on those transport coefficients which enter the hydrodynamic equations of motion. On closer inspection, one finds [12] that the derivation involves net currents which measure the rate of change of conserved quantities in a finite volume and thus require understanding boundary contributions. As a result, Onsager reciprocity constrains both absolute transport coefficients and relative transport coefficients defined relative to the vacuum. Equivalently, it imposes conditions on the derivatives of relative transport coefficients with respect to parameters. To illustrate how this works, let us discuss the constraints imposed by Onsager reciprocity on relative transport coefficients of time-reversal-invariant 2d systems. For the skew-symmetric thermal conductivity κ^A , time-reversal-invariance implies

$$\frac{\partial}{\partial \lambda} \kappa^A = 0, \quad (\text{B1})$$

where λ is a parameter of the Hamiltonian. Thus κ^A can be a function of temperature only. Further, if we treat T as a parameter, then scaling analysis gives

$$\frac{\partial}{\partial T} \frac{\kappa^A}{T} = 0. \quad (\text{B2})$$

Hence $\kappa^A(T) = aT$, where a does not depend on parameters. The parameter a has no physical significance, but it is natural to set it to zero, so that the vacuum has zero thermal Hall conductivity. Thus we reach the standard conclusion that for a system with time-reversal invariance $\kappa^A = 0$.

The case of thermoelectric coefficients is slightly different. Usually one says that Onsager reciprocity requires $\nu_{km} = T^{-1}\eta_{mk}$, which implies $\nu^A + T^{-1}\eta^A = 0$ [9]. Since both ν^A and η^A are relative transport coefficients, one should interpret this as

$$\frac{\partial}{\partial \lambda} (\nu^A + T^{-1}\eta^A) = 0. \quad (\text{B3})$$

Hence $\nu^A + T^{-1}\eta^A$ can depend only on the temperature. If we treat temperature as a parameter, then the scaling analysis gives

$$\frac{\partial}{\partial T} (\nu^A + T^{-1}\eta^A) = 0. \quad (\text{B4})$$

Hence $\nu^A + T^{-1}\eta^A = a$, where a is a constant which is independent of any parameters or temperature and has no physical significance. One can choose it to be zero. Then $\nu^A = -T^{-1}\eta^A$. So for a time-reversal-invariant 2d system there is only one independent skew-symmetric thermoelectric transport coefficient, namely ν^A .

Appendix C: Invariance under Hamiltonian density redefinition

For a given Hamiltonian, there are many ways to define a Hamiltonian density. A typical example of this is the ambiguity in splitting an interaction term between two sites p and q into H_p and/or H_q . In this appendix, we will show that our microscopic formulas for physically observable transport coefficients are independent of the choice of the Hamiltonian density, even though individual terms in the microscopic formulas are not invariant. For some systems this can be used to simplify the microscopic formulas.

1. Invariance of the electric current

Consider the following change of the Hamiltonian density

$$H_p \rightarrow H_p + \sum_{r \in \Lambda} A_{rp}, \quad (\text{C1})$$

where A_{rp} is skew-symmetric in r, p . We want the final Hamiltonian to be $U(1)$ -invariant. Therefore, we have to impose

$$[Q, \sum_{r \in \Lambda} A_{rp}] = 0. \quad (\text{C2})$$

For a general choice of A_{pq} a stronger condition

$$[Q, A_{pq}] = 0, \quad (\text{C3})$$

will not hold. However, one can always redefine A_{pq} (by subtracting the $U(1)$ -non-invariant part) in such a way that (C3) holds without affecting H_p . In the following we will assume this was done and (C3) is true.

Under the transformation (C1) the electric current changes as

$$J_{pq}^N \rightarrow J_{pq}^N + i \sum_{r \in \Lambda} ([A_{rq}, Q_p] - [A_{rp}, Q_q]). \quad (\text{C4})$$

Even though the current density changes, the net current through any section is invariant. Indeed,

$$J^N(\delta f) \rightarrow J^N(\delta f) + \frac{i}{2} \sum_{p, q, r \in \Lambda} ([A_{rq}, Q_p] - [A_{rp}, Q_q]) (f(q) - f(p)), \quad (\text{C5})$$

and the last term is zero since

$$\begin{aligned} & \sum_{p, q, r \in \Lambda} ([A_{rq}, Q_p] - [A_{rp}, Q_q]) (f(q) - f(p)) \\ &= \sum_{p, q, r \in \Lambda} ([A_{rq}, Q_p] + [A_{pr}, Q_q] + [A_{qp}, Q_r]) (f(q) - f(p)) \\ &= \frac{1}{3} \sum_{p, q, r \in \Lambda} ([A_{rq}, Q_p] + [A_{pr}, Q_q] + [A_{qp}, Q_r]) (f(q) - f(p) + f(p) - f(r) + f(r) - f(q)) = 0, \end{aligned} \quad (\text{C6})$$

where we have used (C3) and the skew-symmetry of $[A_{rq}, Q_p] + [A_{pr}, Q_q] + [A_{qp}, Q_r]$.

2. Covariance of the energy current

Let us now consider the effect of the redefinition of the Hamiltonian density on the energy current. Imposing an energy analog of (C2) or (C3)

$$[H, \sum_{r \in \Lambda} A_{rp}] \stackrel{?}{=} 0, \quad \text{or} \quad [H, A_{pq}] \stackrel{?}{=} 0, \quad (\text{C7})$$

is far too restrictive, since it would only allow changes of the Hamiltonian density by conserved quantities. For example, the difference between putting the interaction term between the two sites p and q either into H_p or into H_q corresponds to A_{pq} equal to the interaction term. Obviously, interaction terms are not integrals of motion in general. Because of this we will not impose either of the equations in (C7).

Under the redefinition of the Hamiltonian density (C1) the energy current changes as

$$J_{pq}^E \rightarrow J_{pq}^E + i \sum_{r \in \Lambda} ([A_{rq}, H_p] + [H_q, A_{rp}]), \quad (\text{C8})$$

while the net current transforms as

$$J^E(\delta f) \rightarrow J^E(\delta f) + \frac{i}{2} \sum_{p,q,r \in \Lambda} ([A_{rq}, H_p] + [H_q, A_{rp}]) (f(q) - f(p)). \quad (\text{C9})$$

The last term can be rewritten as

$$\begin{aligned} & \frac{i}{2} \sum_{p,q,r \in \Lambda} ([A_{rq}, H_p] + [H_q, A_{rp}]) (f(q) - f(p)) \\ &= \frac{i}{2} \sum_{p,q,r \in \Lambda} ([A_{rq}, H_p] + [A_{pr}, H_q] + [A_{qp}, H_r]) (f(q) - f(p)) - \frac{i}{2} \sum_{p,q,r \in \Lambda} [A_{qp}, H_r] (f(q) - f(p)) \\ &= \frac{i}{6} \sum_{p,q,r \in \Lambda} ([A_{rq}, H_p] + [A_{pr}, H_q] + [A_{qp}, H_r]) (f(q) - f(p) + f(p) - f(r) + f(r) - f(q)) \\ &\quad - \frac{i}{2} \sum_{p,q \in \Lambda} [H, A_{pq}] (f(q) - f(p)) = -\dot{A}(\delta f), \end{aligned}$$

where we have defined

$$A(\delta f) = \frac{1}{2} \sum_{p,q \in \Lambda} A_{pq} (f(q) - f(p)). \quad (\text{C10})$$

We find that the net energy current transforms as follows under a redefinition of the Hamiltonian density:

$$J^E(\delta f) \rightarrow J^E(\delta f) - \dot{A}(\delta f). \quad (\text{C11})$$

But this should be expected since a redefinition of the energy density changes how we define the energy of sub-regions and therefore should affect the net energy current. Indeed, one can see that (C9) is exactly the transformation needed in order to satisfy the energy conservation law

$$\dot{H}_p = - \sum_{q \in \Lambda} J_{pq}^E \rightarrow \dot{H}_p + \sum_{q \in \Lambda} \dot{A}_{qp} = - \sum_{q \in \Lambda} J_{pq}^E + \sum_{q \in \Lambda} \dot{A}_{qp} \quad (\text{C12})$$

for the new energy density $H_p + \sum_{q \in \Lambda} A_{qp}$. By summing this transformation law over p weighted by a function $f(p)$ with a compact support we find that

$$\dot{H}(f) = -J^E(\delta f) \rightarrow \dot{H}_p + \dot{A}(\delta f) = -J^E(\delta f) + \dot{A}(\delta f), \quad (\text{C13})$$

which reproduces (C11). Here we used an identity

$$\sum_{p,q \in \Lambda} A_{pq} f(q) = \frac{1}{2} \sum_{p,q \in \Lambda} A_{pq} (f(q) - f(p)) = A(\delta f) \quad (\text{C14})$$

which is true for any f with a compact support.

From the above discussion, one can see that energy current is not invariant but covariant under energy density redefinitions. If we choose $f(p)$ to be 1 when p is in some compact set B and zero otherwise, the physical meaning of (C11) is very clear. It corresponds to ambiguities in the energy currents due to interaction terms along the boundary of B . Depending on how we distribute the interaction terms among H_p we can change the energy stored in the region B as well as energy current through its boundary.

3. Invariance of the microscopic formulas for thermoelectric coefficients

In this section we will show that the coefficients ν_{xy} and η_{xy} are invariant under a redefinition of the Hamiltonian density. We will start with skew-symmetric coefficients

$$d\nu^A = \frac{1}{2} d \left(\nu^{\text{Kubo}}(\delta f, \delta g) - \nu^{\text{Kubo}}(\delta g, \delta f) \right) - \beta^2 \mu^N(\delta f \cup \delta g), \quad (\text{C15})$$

$$d\eta^A = \frac{1}{2} d \left(\eta^{\text{Kubo}}(\delta f, \delta g) - \eta^{\text{Kubo}}(\delta g, \delta f) \right) - \beta \mu^N(\delta f \cup \delta g). \quad (\text{C16})$$

Here we defined the Kubo parts as

$$\nu^{\text{Kubo}}(\delta f, \delta g) = \beta^2 \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle \langle J^N(\delta f, t); J^Q(\delta g) \rangle \rangle, \quad (\text{C17})$$

$$\eta^{\text{Kubo}}(\delta f, \delta g) = \beta \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle \langle J^Q(\delta f, t); J^N(\delta g) \rangle \rangle. \quad (\text{C18})$$

Under Hamiltonian density redefinition the Kubo parts transform as

$$\begin{aligned} \nu^{\text{Kubo}}(\delta f, \delta g) &\rightarrow \nu^{\text{Kubo}}(\delta f, \delta g) - \beta^2 \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle \langle J^N(\delta f, t); \dot{A}(\delta g) \rangle \rangle \\ &= \nu^{\text{Kubo}}(\delta f, \delta g) - \beta^2 \langle \langle J^N(\delta f); A(\delta g) \rangle \rangle, \end{aligned} \quad (\text{C19})$$

$$\begin{aligned} \eta^{\text{Kubo}}(\delta f, \delta g) &\rightarrow \eta^{\text{Kubo}}(\delta f, \delta g) - \beta \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle \langle \dot{A}(\delta f, t); J^N(\delta g) \rangle \rangle \\ &= \nu^{\text{Kubo}}(\delta f, \delta g) + \beta \langle \langle A(\delta f); J^N(\delta g) \rangle \rangle, \end{aligned} \quad (\text{C20})$$

where we used properties of the Kubo pairing.

Before finding the variation of the magnetization term it is useful to rewrite it slightly:

$$\begin{aligned}
\mu^N(\delta f \cup \delta g) &= \frac{1}{2} \sum_{p,q \in \Lambda} \left[\frac{1}{3} \sum_{r \in \Lambda} \mu_{pqr}(g_p + g_q + g_r) - \frac{1}{2} \sum_{r \in \Lambda} \mu_{pqr}(g(p) + g(q)) \right] (f(q) - f(p)) \\
&= \frac{1}{2} \sum_{p,q \in \Lambda} \left[\frac{1}{3} \sum_{r \in \Lambda} \mu_{pqr}(g_p + g_q + g_r) - \frac{1}{2} d\langle J_{pq}^N \rangle (g(p) + g(q)) \right] (f(q) - f(p)).
\end{aligned} \tag{C21}$$

Note that one cannot expand the square brackets, since the two resulting sums over p, q will not converge separately.

Let us find the variation of $\frac{1}{2} \langle J_{pq}^N \rangle (g(p) + g(q))$ under a Hamiltonian density redefinition. It reads

$$\begin{aligned}
\frac{1}{2} \langle J_{pq}^N \rangle (g(p) + g(q)) &\rightarrow \frac{1}{2} \langle J_{pq}^N \rangle (g(p) + g(q)) \\
&+ \frac{i}{2} \sum_{r \in \Lambda} \langle [A_{rq}, Q_p] - [A_{rp}, Q_q] \rangle (g(p) + g(q))
\end{aligned} \tag{C22}$$

The last term can be rewritten as follows:

$$\begin{aligned}
\frac{i}{2} \sum_{r \in \Lambda} \langle [A_{rq}, Q_p] - [A_{rp}, Q_q] \rangle (g(p) + g(q)) \\
= \frac{\beta}{2} \sum_{r \in \Lambda} \langle \langle g(p) \dot{Q}_p; A_{rq} \rangle \rangle + \frac{\beta}{2} \sum_{r \in \Lambda} \langle \langle \dot{Q}_p; g(q) A_{rq} \rangle \rangle - (p \leftrightarrow q),
\end{aligned} \tag{C23}$$

where we used the properties of the Kubo pairing. The first term in this expression can be rewritten as

$$\begin{aligned}
\sum_{r \in \Lambda} \langle \langle g(p) \dot{Q}_p; A_{rq} \rangle \rangle - (p \leftrightarrow q) &= -\frac{1}{2} \sum_{s,r \in \Lambda} \langle \langle J_{sp}^N(g(s) + g(p)); A_{rq} \rangle \rangle - (p \leftrightarrow q) \\
&= -\frac{1}{2} \sum_{s,r \in \Lambda} \langle \langle J_{sp}^N(g(s) + g(p)) + J_{ps}^N(g(s) - g(p)); A_{rq} \rangle \rangle - (p \leftrightarrow q) = \langle \langle J^N(\delta g); A_{qp} \rangle \rangle \\
&\quad - \frac{1}{2} \sum_{r,s \in \Lambda} \left[\langle \langle J_{rp}^N(g(r) + g(p)); A_{sq} \rangle \rangle + \langle \langle J_{ps}^N(g(s) - g(p)); A_{rq} \rangle \rangle + 2 \text{ perms} \right],
\end{aligned} \tag{C24}$$

where "2 perms" means the two cyclic permutations in p, q, r . Note that the term in square

brackets is skew-symmetric in p, q, r . The second term can be rewritten as

$$\begin{aligned}
\sum_{r \in \Lambda} \langle \langle \dot{Q}_p; g(q) A_{rq} \rangle \rangle - (p \leftrightarrow q) &= - \sum_{s, r \in \Lambda} \langle \langle J_{sp}^N; g(q) A_{rq} \rangle \rangle - (p \leftrightarrow q) \\
&= -\frac{1}{2} \sum_{s, r \in \Lambda} \langle \langle J_{sp}^N; A_{rq}(g(q) + g(r)) + A_{qr}(g(r) - g(q)) \rangle \rangle - (p \leftrightarrow q) = \langle \langle J_{pq}^N; A(\delta g) \rangle \rangle \\
&\quad - \frac{1}{2} \sum_{s, r \in \Lambda} \left[\langle \langle J_{sp}^N; A_{rq}(g(q) + g(r)) \rangle \rangle + \langle \langle J_{rp}^N; A_{qr}(g(r) - g(q)) \rangle \rangle + 2 \text{ perms} \right]. \quad (\text{C25})
\end{aligned}$$

Note that term in square brackets is skew-symmetric in p, q, r

By combining equations (C21-C25) we find that the magnetization contribution changes under a redefinition of the Hamiltonian density as follows:

$$\begin{aligned}
\mu^N(\delta f \cup \delta g) \rightarrow \mu^N(\delta f \cup \delta g) &- \frac{\beta}{2} d \langle \langle J^N(\delta f); A(\delta g) \rangle \rangle + \frac{\beta}{2} d \langle \langle J^N(\delta g); A(\delta f) \rangle \rangle \\
&+ \frac{1}{2} \sum_{p, q, r \in \Lambda} C_{pqr}(f(q) - f(p)), \quad (\text{C26})
\end{aligned}$$

where C_{pqr} is a skew-symmetric function of p, q, r which is combination of skew-symmetric parts (and their derivatives) in the right-hand sides of Eqs. (C21-C25). Due to its skew-symmetry we find that

$$\frac{1}{2} \sum_{p, q, r \in \Lambda} C_{pqr}(f(q) - f(p)) = \frac{1}{6} \sum_{p, q, r \in \Lambda} C_{pqr}(f(q) - f(p) + f(p) - f(s) + f(s) - f(q)) = 0. \quad (\text{C27})$$

We see that the variation of the magnetization exactly compensates the variation of the Kubo parts. Thus the skew-symmetric parts of the thermoelectric tensors are invariant under a redefinition of the Hamiltonian density.

Now let us consider the symmetric parts

$$\nu_{xy}^S = \frac{1}{2} \left(\nu^{\text{Kubo}}(\delta f, \delta g) + \nu^{\text{Kubo}}(\delta g, \delta f) \right) + \beta U(\delta f, \delta g), \quad (\text{C28})$$

$$\eta_{xy}^S = \frac{1}{2} \left(\eta^{\text{Kubo}}(\delta f, \delta g) + \eta^{\text{Kubo}}(\delta g, \delta f) \right) - U(\delta f, \delta g). \quad (\text{C29})$$

The variation of Kubo parts were already determined before, so we focus on the transformation of U . Under (C1) it transforms as follows:

$$U(\delta f, \delta g) \rightarrow U(\delta f, \delta g) + \frac{i}{4} \sum_{p, q \in \Lambda} \langle [\partial A_q, Q_p] + [\partial A_p, Q_q] \rangle (f(q) - f(p))(g(q) - g(p)). \quad (\text{C30})$$

We can rewrite this equation by noticing that

$$\frac{i}{2} \langle [\partial A_q, Q_p] + [\partial A_p, Q_q] \rangle (g(q) - g(p)) = -\frac{\beta}{2} \langle \langle g(p) \dot{Q}_p; \partial A_q \rangle \rangle + \frac{\beta}{2} \langle \langle \dot{Q}_p; \partial g(q) A_q \rangle \rangle - (p \leftrightarrow q). \quad (\text{C31})$$

Then using eqs. (C24, C25) we find

$$U(\delta f, \delta g) \rightarrow U(\delta f, \delta g) + \frac{\beta}{2} \langle \langle J^N(\delta f); A(\delta g) \rangle \rangle + \frac{\beta}{2} \langle \langle J^N(\delta g); A(\delta f) \rangle \rangle \quad (\text{C32})$$

We see that the variation of this term cancels the variations of the Kubo parts.

One can do the same checks for the thermal Hall conductivity and verify that the microscopic formula derived in [5] is invariant under a redefinition of the Hamiltonian density. To linear order in A_{pq} all the manipulations are almost the same except for the replacement $Q_p \rightarrow H_p$ and $J^N \rightarrow J^E$.

Appendix D: Thermoelectric coefficients for free fermions

1. Definitions and correlation functions

In this appendix we will specialize our microscopic formulas for coefficients ν and η to free fermionic systems. The Hamiltonian is taken to be

$$H = \sum_{p,q \in \Lambda} a_p^\dagger h(p, q) a_q, \quad (\text{D1})$$

where an infinite matrix $h(p, q)$ is Hermitian $h(p, q)^* = h(q, p)$, and a_p^\dagger, a_p are fermionic creation-annihilation operators satisfying the standard anti-commutation relations

$$a_p a_q^\dagger + a_q^\dagger a_p = \delta_{p,q}, \quad a_p a_q + a_q a_p = a_p^\dagger a_q^\dagger + a_q^\dagger a_p^\dagger = 0. \quad (\text{D2})$$

We define the Hamiltonian density on site p to be

$$H_p = \frac{1}{2} \sum_{m \in \Lambda} (a_p^\dagger h(p, m) a_m + a_m^\dagger h(m, p) a_p). \quad (\text{D3})$$

The charge operator on site p is defined as

$$Q_p = a_p^\dagger a_p. \quad (\text{D4})$$

The electric current can be found from the conservation equation:

$$J_{pq}^N = i(a_q^\dagger h(q, p) a_p - a_p^\dagger h(p, q) a_q). \quad (\text{D5})$$

The net current through a section defined by $\delta f(p, q) = f(q) - f(p)$ is

$$J(\delta f) = -i a^\dagger [h, f] a,$$

where a bounded function $f \in \ell^2(\Lambda)$ is understood as an operator acting on the one-particle Hilbert space $\ell^2(\Lambda)$ by multiplication. Summation over sites is implicit.

The energy current operator is

$$J_{pq}^E = \frac{-i}{4} \sum_{m \in \Lambda} (a_p^\dagger h(p, q) h(q, m) a_m - a_q^\dagger h(q, p) h(p, m) a_m \\ - a_m^\dagger h(m, q) h(q, p) a_q + a_m^\dagger h(m, p) h(p, q) a_q \\ + a_p^\dagger h(p, m) h(m, q) a_q - a_q^\dagger h(q, m) h(m, p) a_p). \quad (\text{D6})$$

The net energy current is

$$J^E(\delta f) = -\frac{i}{2} a^\dagger [h^2, f] a.$$

The state of the system at a temperature $T = 1/\beta$ is defined via Wick's theorem and Gibbs distribution

$$\langle a_p(t) a_q^\dagger \rangle = \left\langle p \left| \frac{e^{-iht}}{1 + e^{-\beta h}} \right| q \right\rangle, \quad (\text{D7})$$

$$\langle a_p(t)^\dagger a_q \rangle = \left\langle q \left| \frac{e^{iht}}{1 + e^{\beta h}} \right| p \right\rangle, \quad (\text{D8})$$

where $a_p(t)$ are operators in the Heisenberg picture.

Using these formulas we find

$$\langle J^N(\delta f, t) J^N(\delta g) \rangle = -\text{Tr} \left([h, f] \frac{e^{-iht}}{1 + e^{-\beta h}} [h, g] \frac{e^{iht}}{1 + e^{\beta h}} \right),$$

where the trace is over the 1-particle Hilbert space $\ell^2(\Lambda)$, and the functions $f : \Lambda \rightarrow \mathbb{R}$ and $g : \Lambda \rightarrow \mathbb{R}$ are operators on this Hilbert space. The operators $[h, f]$ and $[h, g]$ have support on a vertical strip and a horizontal strip, respectively.

Switching to the energy basis, substituting $t \rightarrow t - i\tau$, and integrating from 0 to β over τ we find

$$\langle \langle J^N(\delta f, t); J^N(\delta g) \rangle \rangle = \frac{-1}{\beta} \sum_{n, m} \langle n | [h, f] | m \rangle \langle m | [h, g] | n \rangle e^{i(\varepsilon_n - \varepsilon_m)t} \frac{e^{\beta \varepsilon_n} - e^{\beta \varepsilon_m}}{(1 + e^{\beta \varepsilon_n})(1 + e^{\beta \varepsilon_m})(\varepsilon_n - \varepsilon_m)},$$

where ε_n are 1-particle Hamiltonian energy eigenvalues.

Multiplying this by e^{-st} and integrating over t , we arrive at

$$\sigma_{xy} = i \lim_{s \rightarrow 0} \sum_{n, m} \frac{\langle n | [h, f] | m \rangle \langle m | [h, g] | n \rangle \mathfrak{f}(\varepsilon_n) - \mathfrak{f}(\varepsilon_m)}{\varepsilon_n - \varepsilon_m + is} \frac{1}{\varepsilon_n - \varepsilon_m},$$

where $\mathfrak{f}(\varepsilon) = \frac{1}{1+e^{\beta(\varepsilon)}}$ is the Fermi-Dirac distribution. We absorb the chemical potential into a shift of the Hamiltonian.

The above expressions assume a discrete energy spectrum and thus can only be used for finite-volume systems. To get an expression applicable to infinite-volume systems, let us rewrite it in terms of the one-particle Green's functions $G_{\pm}(z) = 1/(z - h \pm i0)$. Some of the useful formulas are

$$\begin{aligned}\langle a^\dagger A a \rangle &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left([G_+ - G_-] A \right), \\ -\beta \langle \langle a^\dagger A a; a^\dagger B a \rangle \rangle &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left([G_+ - G_-] A G_+ B + G_- A [G_+ - G_-] B \right) \\ &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left(G_+ A G_+ B - G_- A G_- B \right),\end{aligned}\tag{D9}$$

where we have dropped z for $G_{\pm}(z)$. Here A and B are operators acting on the one-particle Hilbert space, and in the second formula we assumed in addition that their average is zero: $\langle a^\dagger A a \rangle = \langle a^\dagger B a \rangle = 0$. Note also that

$$h G_{\pm} = G_{\pm} h = z G_{\pm} - 1, \quad [G_{\pm}, A] = G_{\pm} [h, A] G_{\pm}.$$

Using this notation the formula for the electric conductivity takes the form

$$\sigma_{xy} = -\frac{1}{2\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \{ [h, f] G_+^2 [h, g] (G_+ - G_-) - [h, f] (G_+ - G_-) [h, g] G_-^2 \}, \tag{D10}$$

where the integration is over the real axis in the z -plane.

2. Magnetization term

The magnetization differential for an arbitrary deformation dh of the 1-particle Hamiltonian is given by

$$\mu^N(\delta f \cup \delta g) = \frac{1}{4\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left(G_+ dh G_+ \left\{ [h, f] G_+ [h, g] - [h, g] G_+ [h, f] \right\} \right) - (G_+ \rightarrow G_-). \tag{D11}$$

For temperature variations this expression can be simplified to

$$\begin{aligned}\tau^N(\delta f \cup \delta g) &= \frac{1}{4\pi} \int_{-\infty}^{\infty} dz \text{Tr} \left(\mathfrak{f}(z) (G_+ - G_-) [h^2, f] G_-^2 [h, g] - \mathfrak{f}(z) (G_+ - G_-) [h^2, g] G_+^2 [h, f] \right. \\ &\quad \left. + \mathfrak{f}'(z) (G_+ - G_-) h [h, g] G_+ [h, f] + \mathfrak{f}'(z) (G_+ - G_-) h [h, g] G_- [h, f] \right) - (f \leftrightarrow g). \end{aligned} \tag{D12}$$

These expressions are needed only for the evaluation of skew-symmetric parts of the thermoelectric coefficients.

3. U -term

Let us study the term (51) for free fermionic system. In this case the relevant many-body operators become

$$([Q_p, H_q] + [Q_q, H_p]) = a^\dagger [h, \delta_p \delta_q] a, \quad (\text{D13})$$

where δ_p is a Kronecker delta function equal 1 on site p and 0 on all other sites. A product of two delta functions enforces $q = p$ in the summation over p and q . Since U also involves a factor of $(g(p) - g(q))(f(p) - f(q))$, $U(\delta f, \delta g)$ vanishes for systems of free fermions.

More generally, one can consider a system of fermions with only density-dependent interactions. Namely, suppose we allow the following interaction term in the Hamiltonian (D1):

$$H^{\text{int}} = \sum_{p_1, \dots, p_n \in \Lambda} V(p_1, \dots, p_n) Q_{p_1} \dots Q_{p_n}, \quad (\text{D14})$$

where $V(p_1, \dots, p_n)$ is a function of n sites which describes the potential energy of many-body interaction and decays rapidly when the points p_1, \dots, p_n are far from each other. One can see that this term will leave eq. (D13) unaffected since Q_p commute with each other. We conclude that for fermionic system with only density-dependent interactions there is no correction originating from U to the symmetric thermoelectric coefficients provided H_p is chosen in the manner explained above.

4. Skew-symmetric part

Consider the variation of the Kubo parts (C17, C18) of the skew-symmetric thermoelectric coefficients under a rescaling of the Hamiltonian: $dh = h d\lambda_0$. We get

$$\begin{aligned} d\nu_{\text{Kubo}}^A &= \beta d\eta_{\text{Kubo}}^A(\delta f \cup \delta g) = \frac{d\lambda_0}{4\pi} \int_{-\infty}^{\infty} dz \text{Tr} \left(\mathfrak{f}(z)(G_+ - G_-)[h^2, f]G_-^2[h, g] \right. \\ &\quad - \mathfrak{f}(z)(G_+ - G_-)[h^2, g]G_+^2[h, f] + \mathfrak{f}'(z)(G_+ - G_-)h[h, g]G_+[h, f] + \mathfrak{f}'(z)(G_+ - G_-)h[h, g]G_-[h, f] \\ &\quad \left. - 2\mathfrak{f}'(z)h^2(G_+ - G_-)[h, f]G_+^2[h, g] + 2\mathfrak{f}'(z)h^2(G_+ - G_-)[h, g]G_-^2[h, f] \right) - (f \leftrightarrow g). \quad (\text{D15}) \end{aligned}$$

Summing up this contributions with the magnetization contribution gives

$$\frac{d\nu^A}{dT} = \frac{d}{dT} \left(\frac{\eta^A}{T} \right) = \frac{1}{2\pi T^2} \int_{-\infty}^{\infty} dz \mathfrak{f}'(z) z^2 \text{Tr} \left((G_+ - G_-)[h, f] G_+^2[h, g] \right. \\ \left. - (G_+ - G_-)[h, g] G_-^2[h, f] - (f \leftrightarrow g) \right). \quad (\text{D16})$$

Integrating over the temperature and using the formula

$$\int_T^{\infty} \frac{dT}{T^2} \mathfrak{f}'(z) = \frac{c_1(\mathfrak{f}(z)) - \log 2}{z^2}, \quad (\text{D17})$$

where

$$c_1(x) = \int_0^x dt \log \left(\frac{1-t}{t} \right) = -x \log x - (1-x) \log(1-x), \quad (\text{D18})$$

gives

$$\nu^A = \frac{\eta^A}{T} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dz c_1(\mathfrak{f}(z)) \text{Tr} \left((G_+ - G_-)[h, f] G_+^2[h, g] \right. \\ \left. - (G_+ - G_-)[h, g] G_-^2[h, f] - (f \leftrightarrow g) \right). \quad (\text{D19})$$

Here we normalized the thermoelectric coefficients to be 0 in the infinite-temperature state. Note that since in the limit $T \rightarrow 0$ the Fermi-Dirac distribution $\mathfrak{f}(z)$ becomes a step-function, and since $c_1(0) = c_1(1) = 0$, both $\nu^A(T)$ and $\eta^A(T)/T$ vanish at $T = 0$ regardless of the choice of the Hamiltonian h .

5. Symmetric part

Symmetric parts of transverse thermoelectric coefficients are

$$\nu_{xy}^S = -\frac{\beta}{8\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \{ [h, f] G_+^2[h^2, g] (G_+ - G_-) - [h, f] (G_+ - G_-) [h^2, g] G_-^2 \} + (f \leftrightarrow g), \\ \eta_{xy}^S = -\frac{1}{8\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \{ [h^2, f] G_+^2[h, g] (G_+ - G_-) - [h^2, f] (G_+ - G_-) [h, g] G_-^2 \} + (f \leftrightarrow g).$$

As explained in the body of the paper, longitudinal parts are given by the same formulas with a more general choice of the functions f, g .

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